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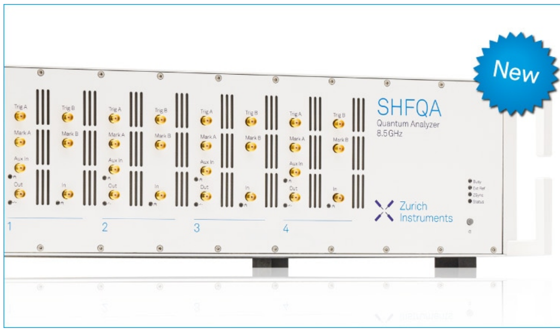

Geometric Representation of Polycrystalline Material Texture by Axis-Angle Parametrization

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Abstract. Texture is the preferential orientation of crystallographic axes in polycrystal. For its mathematical modeling, the orientation distribution function of the crystallographic axes is used. Traditionally, the orientation distribution function is written with the help of directional cosine matrices, Miller indices or Euler-Krylov angles. Recently, texture has increasingly often been described using quaternions, Rodrigues parameters and the vector space of axis-angle parameters. Axis-angle parameters allow us to describe all possible rotations of the *SO*(3) group, which corresponds to all possible orientations of crystallographic axes in polycrystalline materials. The *SO*(3) group is a set of rotations to all possible angles around all possible axes given by all vectors of the unit sphere. The set of such rotations corresponds to points set on a ball of radius π in three-dimensional Euclidean space. The description of the crystallographic texture using axis-angle parameters made it possible to visualize the distribution of crystallographic axes and obtain a new geometric representation of the texture.

INTRODUCTION

To determine elastic, plastic, strength and other physical and mechanical properties of polycrystalline materials, it is necessary to study the preferential orientation of crystallographic axes, termed texture. Texture is shaped under various modes of thermomechanical processing for polycrystalline materials and has a significant effect on the anisotropy of these properties. Various systems of variables for description orientations of crystallographic axes in a polycrystalline material are used. These systems can be represented with the help of directional cosine matrices, Miller indices, Euler-Krylov angles, quaternions, Rodrigues parameters and so on. Each of these systems has its advantages and disadvantages in solving a particular problem. Various modifications and combinations of these systems are also used.

In texture analysis, problems of Euler-Krylov angles are most widely used. Analysis of the texture in the Euler-Krylov angle parameters is represented by a variety of different space cross-sections. It is possible to obtain the distribution of movable axes throughout this space. There is no possibility of obtaining a quantitative characteristic of the distribution of these axes in a limited volume of the space. For the quantitative description of the crystallographic texture, in this case, the orientation distribution function and its expansion in terms of generalized spherical functions is used. Obtaining the orientation distribution function is a separate task of texture analysis. At an intermediate stage of describing a uniform probability of orientation distribution of crystallographic axes in a limited space volume, the Euler-Krylov angular distribution density is used, which is defined by

$$f(\psi,\vartheta,\varphi)=\frac{1}{8\pi^2}\sin\vartheta\,,\ 0\le\psi\le 2\pi\,,\ 0\le\vartheta\le\pi\,,\ 0\le\varphi\le 2\pi\,.$$

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In recent years, quantitative characteristics of random distributions of crystallographic axes through the axis-angle parameters have been considered taking into account a wide application of quaternion methods for rotation description. Texture components and their volume fraction cannot be visualized by Miller indices or quaternions. The paper gives their geometric representation in terms of axis-angle parameters to visualize crystallographic texture. Axis-angle parameters determine Rodrigues parameters. Rodrigues parameters, in turn, determine the orientation of crystallographic axes by unit quaternion coordinates.

DISTRIBUTION OF CRYSTALLOGRAPHIC AXES ON THE *SO*(3) GROUP

The position of a single crystal can be uniquely determined by the quaternion $\boldsymbol{\lambda} = \lambda_0 + \lambda_1 i_1 + \lambda_2 i_2 + \lambda_3 i_3$ with a unit norm $\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = 1$. Such quaternions form a group $Sp(1)$ ($SO(3) \approx Sp(1) \pm 1$). The three-dimensional sphere of unit radius S^3 is a two-sheeted cover for the $SO(3)$ group [1]. It means that the quaternions λ_i and $-\lambda_i$ correspond to the same element of $SO(3)$ [2]. As shown in [3], the $SO(3)$ group can be represented as a set of rotations to all possible angles $0 \le \chi \le \pi$ round all possible axes. These axes are given by all vectors (α, β), $0 \le \alpha \le \pi$, $0 \le \beta \le 2\pi$. The set of all such rotations corresponds to points inside the ball of radius π in the three-dimensional Euclidean space [4]. On the surface of this ball, it is necessary to identify opposite points, since rotation by an angle π around the vector $\boldsymbol{\omega}$ coincides with rotation by an angle π, about the vector $-\boldsymbol{\omega}$. There are no other coinciding rotations on the ball. The mapping of $SO(3)$ onto the ball of radius π is not bijective. This fact does not serve as an obstacle for purposes of modeling random distributions. The measure of points set on the ball surface is zero. The quaternion $\boldsymbol{\lambda}$ [5] for the description the rotation of movable axes using axis-angle parameters is

$$\boldsymbol{\lambda} = \cos\frac{\chi}{2} + \sin\frac{\chi}{2}\omega_1(\alpha,\beta)i_1 + \sin\frac{\chi}{2}\omega_2(\alpha,\beta)i_2 + \sin\frac{\chi}{2}\omega_3(\alpha,\beta)i_3 .$$

Hence the uniform distribution of movable axes in the space part with boundaries as the angle γ corresponds to the homogeneous ball of radius γ ($0 \le \gamma \le \pi$) in the three-dimensional Euclidean space. The point position in this sphere is defined by equalities using spherical coordinates,

$$x_1 = \chi\omega_1 = \chi\sin\alpha\cos\beta\,,\ x_2 = \chi\omega_2 = \chi\sin\alpha\sin\beta\,,\ x_3 = \chi\omega_3 = \chi\cos\alpha\,,\ 0 \le \alpha \le \pi\,,\ 0 \le \beta \le 2\pi\,,\ 0 \le \chi \le \gamma\,.$$

These coordinates, for each of the angles χ, α, β, determine the corresponding point inside the ball of radius π, and this point corresponds to a certain position of crystallographic axes (Fig. 1).

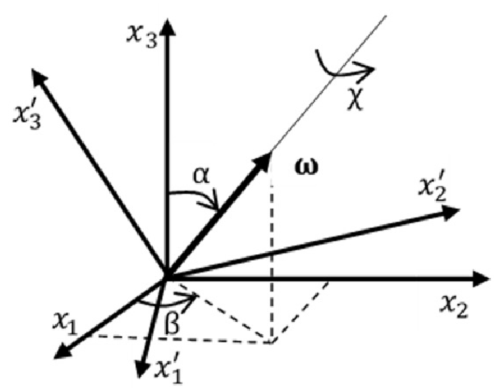


FIGURE 1. The position of the crystallographic coordinate system using the axis-angle parameters

The density of the distribution of the angles χ, α, β corresponding to the uniform distribution of movable axes can be obtained using the following theorem [6].

Theorem. Let the functions $x_1(u_1, u_2,\ldots, u_m)$, $x_2(u_1, u_2,\ldots, u_m)$,…, and $x_n(u_1, u_2,\ldots, u_m)$, where $(u_1, u_2,\ldots, u_m) \in D$ define a smooth regular m – dimensional surface in the n – dimensional Euclidean space. Then the distribution density of the values of the parameters $u_1, u_2, \ldots, u_m$, which determines the uniform distribution of points on this surface, is determined by the function

$$f(u_1, u_2, \ldots, u_m) = \begin{cases} \dfrac{\sqrt{g}}{\iiint_D \ldots \int \sqrt{g}\, du_1 du_2 \ldots du_m}, & (u_1, u_2, \ldots, u_m) \in D; \\ 0, & (u_1, u_2, \ldots, u_m) \notin D. \end{cases}$$

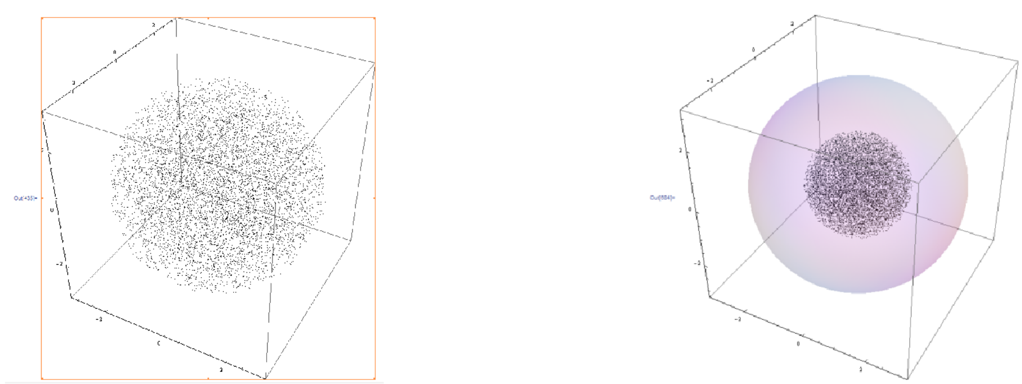
We can generate the values of the parameters $u_1, u_2, \ldots, u_m$ using the function $f(u_1, u_2, \ldots, u_m)$ by the generalized Neumann method and obtain a uniform distribution of points on the surface.

DENSITY OF ISOTROPIC DISTRIBUTION

The assertion of this theorem remains valid also in the case when $m = n$, this is a smooth mapping of a finite-dimensional space onto itself. Then, the density $f(\alpha, \beta, \chi)$ of the joint distribution of the angles α, β, χ determines a uniform distribution of points in the ball of radius γ. The uniform distribution of movable axes in the bounded volume of the orientation space is defined by the equality

$$f(\alpha, \beta, \chi) = \begin{cases} \dfrac{3\chi^2 \sin\alpha}{4\pi\gamma^3}, & (\alpha, \beta, \gamma) \in D,\ D = [0 \le \alpha \le \pi, 0 \le \beta \le 2\pi, 0 \le \chi \le \gamma]; \\ 0, & (\alpha, \beta, \gamma) \notin D. \end{cases}$$

We substitute the angle γ in this function by angles equal to π and $\pi/2$ and obtain a uniform distribution of points in the ball of radii equal to π and $\pi/2$. We performed a numerical experiment in the Mathematica 7 package using the Neumann method. The result of the experiment is shown in Fig. 2. Both distributions correspond to the isotropic distribution of crystallographic axes. The first distribution is defined on the entire orientation space. The second distribution is defined in the space with boundaries as the solid angle $\pi/2$.



(a) (b)

FIGURE 2. The "point clouds" corresponding to the uniform and isotropic distributions of 10,000 orientations: the ball of radius π (a); the ball of $\pi/2$ (b)

DENSITY OF ANISOTROPIC NORMAL DISTRIBUTION

From what has been said above, it follows that a non-uniform distribution of points in the ball corresponds to a certain uneven distribution of movable axes. In texture analysis, normal distributions are used on the $SO(3)$ group [7]. We obtain the density of the normal distribution of the crystallographic axes on the $SO(3)$ group using the axis-angle parameters in the form

$$f(\alpha,\beta,\chi)=\frac{e^{-\sigma\chi^2}\sin\alpha}{4\pi\int_0^\pi e^{-\sigma\chi^2}d\chi},\ (\alpha,\beta,\gamma)\in D,\ D=[0\le\alpha\le\pi,0\le\beta\le 2\pi,0\le\chi\le\gamma].$$

The result for a numerical experiment on the distribution of 10,000 points in the ball using this density for normal distribution is shown in Fig. 3. This distribution corresponds to a "points cloud" in the ball of radius π, whose density varies according to the normal law.

Another example is given. The anisotropic distribution of crystallographic axes on the *SO*(3) group using axis-angle parameters is considered. The density is equal to

$$f(\alpha,\beta,\chi)=\frac{e^{-\sigma\chi^2}\sin\alpha}{2\pi(\cos\delta_1-\cos\delta_2)\int_0^\pi e^{-\sigma\chi^2}d\chi},\ (\alpha,\beta,\gamma)\in D,\ D=[0\le\alpha\le\pi,0\le\beta\le 2\pi,0\le\chi\le\gamma].$$

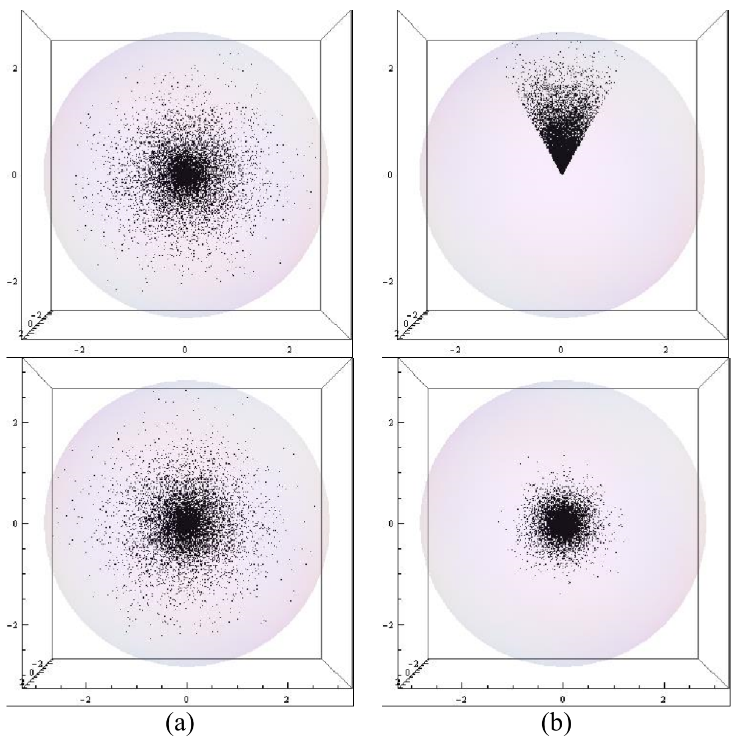


FIGURE 3. "Point clouds" for normal isotropic (left) and anisotropic (right) distributions of 10,000 orientations when σ=0.5, δ_1=0, δ_2=π/4, 0≤α≤π/4. The ball is of radius π. The viewpoints are {5,0,0} a) and {0,0,5} (b)

The result of the numerical experiment on the distribution of 10,000 points in the ball using the obtained density of normal distribution in space with boundaries as the solid angle is shown in Fig. 3.

CONCLUSION

The paper gives a geometric representation of crystallographic texture for polycrystalline materials. The uniform distribution of crystallographic movable axes inside a certain limited space is visualized by the Neumann method. The "point clouds" corresponding to crystallographic directions are constructed in the ball of radius π. The density of their distribution changes according to the normal law. The distributions of crystallographic axes corresponding to both the isotropic and anisotropic state of the polycrystalline material have been considered. This fact is clearly reflected in the shape of the "point clouds".

This paper has proposed a method for generating a uniform distribution of movable axes using axis-angle parameters. This method can be implemented despite the fact that the mapping of *SO*(3) onto the ball is not bijective. This is due to the fact that the probability of points hitting the ball surface is zero. There are no corresponding points in the resulting sample.

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